L Number	Hits	Search Text	DB	Time stamp
1	1251	((544/320) or (544/243)).CCLS.	USPAT; US-PGPUB; EPO; JPO; DERWENT	2003/04/02 07:51
2	1922096	2002.py. or 2003.py.	USPAT; US-PGPUB; EPO; JPO; DERWENT	2003/04/02 07:51
3	65	(((544/320) or (544/243)).CCLS.) and (2002.py. or 2003.py.)	USPAT; US-PGPUB; EPO; JPO; DERWENT	2003/04/02 07:51

L Number	Hits	Search Text	DB	Time stamp
1	1225	((544/320) or (544/243)).CCLS.	USPAT; US-PGPUB; EPO; JPO; DERWENT	2002/11/14 10:54

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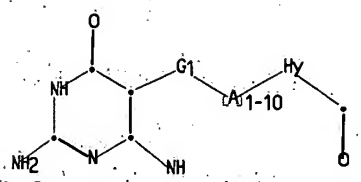

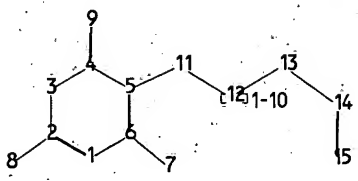

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7 8 9 11 12 13 14 15
ring nodes :
1 2 3 4 5 6
chain bonds :
2-8 4-9 5-11 6-7 11-12 12-13 13-14 14-15
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
1-2 1-6 2-3 2-8 3-4 4-5 4-9 5-6 5-11 6-7 11-12 12-13 13-14 14-15
isolated ring systems :
containing 1 :

G1:S,Se

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 11:CLASS
12:CLASS 13:Atom 14:CLASS 15:CLASS

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L1      STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1                STR
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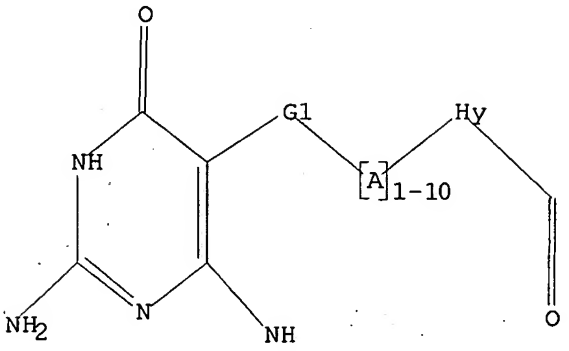


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G1 S,Se

...

Structure attributes must be viewed using STN Express query preparation.


=> s l1 sss sam
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SAMPLE SCREEN SEARCH COMPLETED -     14 TO ITERATE

100.0% PROCESSED      14 ITERATIONS                                1 ANSWERS
SEARCH TIME: 00.00.02

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:           56 TO      504
PROJECTED ANSWERS:               1 TO       80

L2            1 SEA SSS SAM L1

=> s l1 sss ful
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100.0% PROCESSED     201 ITERATIONS                               16 ANSWERS
SEARCH TIME: 00.00.09

L3           16 SEA SSS FUL L1

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L4            5 L3

=> d l4 1-5 bib,ab,hitstr
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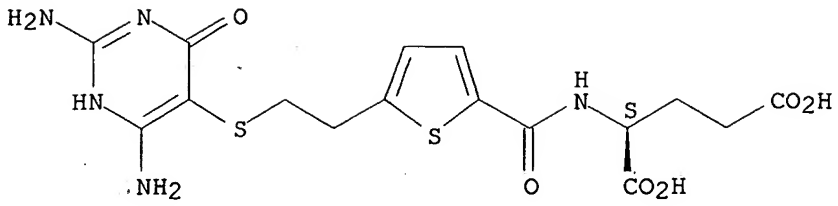
L4 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2002 ACS
AN 1998:484508 CAPLUS
DN 129:211256
TI Super in vitro synergy between inhibitors of dihydrofolate reductase and inhibitors of other folate-requiring enzymes: the critical role of polyglutamylation
AU Faessel, Helene M.; Slocum, Harry K.; Jackson, Robert C.; Boritzki, Theodore J.; Rustum, Youcef M.; Nair, M. G.; Greco, William R.
CS Grace Cancer Drug Center, New York State Department of Health, Roswell Park Cancer Institute, Buffalo, NY, 14263, USA
SO Cancer Research (1998), 58(14), 3036-3050
CODEN: CNREA8; ISSN: 0008-5472
PB American Association for Cancer Research
DT Journal
LA English
AB The combined action among polyglutamylatable and nonpolyglutamylatable antifolates, directed against dihydrofolate reductase (DHFR), glycinamide ribonucleotide formyltransferase (GARFT), 5-aminoimidazole-4-carboxamide ribonucleotide formyltransferase (AICARFT), and thymidylate synthase (TS), in human ileocecal HCT-8 cells was examd. in a 96-well plate growth inhibition assay (96-h continuous drug exposure). An interaction parameter, .alpha., was estd. for each of 95 expts. by fitting a seven-parameter model to data with weighted nonlinear regression. In a representative expt., raising the folic acid concn. in the medium dramatically increased the Loewe synergy for the combination of trimetrexate (TMTX) and the GARFT inhibitor AG2034 (from a mean .alpha. .+-. SE of 1.50 at 2.3 .mu.M folic acid to 146 at 78 .mu.M folic acid). Enhancements were also found for combinations of TMTX with the GARFT inhibitors AG2032, Lometrexol, and LY309887, the AICARFT inhibitor AG2009, and the TS inhibitors LY231514 and Tomudex but not with the GARFT inhibitor LL95509 or with the TS inhibitors AG337, ZD9331, and BW1843U89. Replacing TMTX with methotrexate in two-drug mixts. decreased the intensity of Loewe synergy. Examn. of isobolograms at different effect levels revealed informative reproducible changes in isobol patterns. No two-drug combinations among inhibitors of GARFT, AICARFT, and TS exhibited Loewe synergy at either 2.3 or 78 .mu.M folic acid. Thus, the ideal requirement for the folic acid-enhanced synergy is that a nonpolyglutamylatable DHFR inhibitor be combined with a polyglutamylatable inhibitor of another folate-requiring enzyme. A hypothesis to explain this general phenomenon involves the crit. role of folylpoly-.gamma.-glutamate synthetase and the effect of the DHFR inhibitor in decreasing the protection by folic acid of cells to the other antifolates.
IT **160743-73-7**, AG 2009
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(super in vitro synergy between inhibitors of dihydrofolate reductase and inhibitors of other folate-requiring enzymes and crit. role of polyglutamylation)
RN 160743-73-7 CAPLUS
CN L-Glutamic acid, N-[[5-[2-[(2,6-diamino-1,4-dihydro-4-oxo-5-pyrimidinyl)thio]ethyl]-2-thienyl]carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



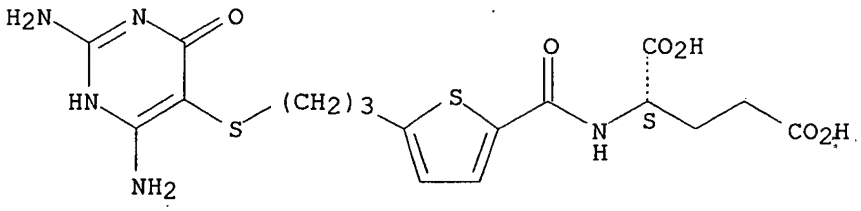
L4 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2002 ACS
AN 1998:236275 CAPLUS
DN 128:283082
TI Preparation of antiproliferative substituted 5-thiapyrimidinone and 5-selenopyrimidinone compounds
IN Varney, Michael D.; Romines, William H.; Palmer, Cynthia L.; Deal, Judith G.
PA Agouron Pharmaceuticals, Inc., USA
SO U.S., 23 pp., Cont.-in-part of U.S. Ser. No. 991,259, abandoned.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 3

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 5739141	A	19980414	US 1995-448556	19950607
	WO 9413295	A1	19940623	WO 1993-US11795	19931210
	W: AT, AU, BB, BG, BR, BY, CA, CH, CZ, DE, DK, ES, FI, GB, HU, JP, KP, KR, KZ, LK, LU, LV, MG, MN, MW, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SK, UA, US, UZ, VN				
	RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
	US 5945427	A	19990831	US 1998-3163	19980106
	US 6207670	B1	20010327	US 2000-588654	20000607
	US 2001018443	A1	20010830	US 2001-782284	20010214
	US 6323210	B2	20011127		
PRAI	US 1992-991259	B2	19921216		
	WO 1993-US11795	W	19931210		
	US 1995-448556	A3	19950607		
	US 1998-3163	A3	19980106		
	US 1999-307595	A3	19990510		
	US 2000-588654	A3	20000607		

OS MARPAT 128:283082
AB The present invention is directed to title derivs. I [A = S, Se; Z = (un)substituted spacer group contg. 1-10 C, O, S, N, or P atoms, (un)substituted, (non)fused polycyclic or heterocyclic group, or a combination of both; R1, R2 = independently H, C1-6 alkyl, or other readily lyzable, preferably hydrolyzable group; R3 = H, (un)branched (a)cyclic C1-6 alkyl optionally contg. one or more halo , OH, or amino groups], or pharmaceutically acceptable salts thereof, which are useful as inhibitors of the enzymes glycinamide ribonucleotide formyl transferase (GARFT) and amino imidazole carboxamide ribonucleotide formyl transferase (AICARFT), pharmaceutical compns. contg. these derivs., and methods of using these derivs. The present invention is also directed to intermediates useful for prepg. these derivs. and methods of prepg. these intermediates. Thus, thiapyrimidinone II, prepd. in several steps from 5-bromo-3-methylthiophene-2-carboxylic acid, propargyl alc., di-Et L-glutamate, and 5-bromo-2,6-diamino-4(3H)-pyrimidinone, inhibited GARFT with Ki = 0.008 .mu.M.
IT **160743-67-9P 160743-70-4P 160743-71-5P**
160743-72-6P 160743-73-7P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of substituted thiapyrimidinone and selenopyrimidinone derivs. as antiproliferative agents)
RN 160743-67-9 CAPLUS
CN L-Glutamic acid, N-[[5-[3-[(2,6-diamino-1,4-dihydro-4-oxo-5-

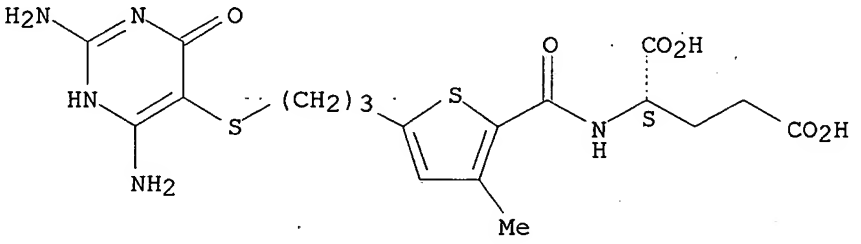
pyrimidinyl)thio]propyl]-2-thienyl]carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



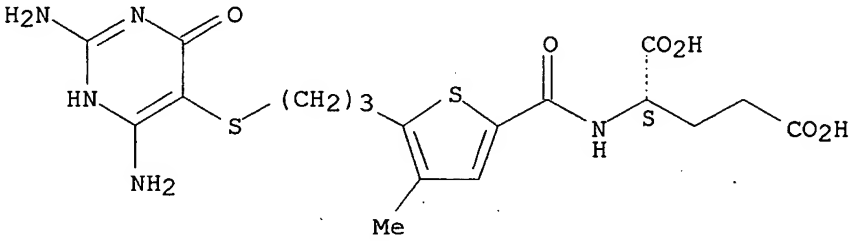
RN 160743-70-4 CAPLUS
CN L-Glutamic acid, N-[[5-[3-[(2,6-diamino-1,4-dihydro-4-oxo-5-pyrimidinyl)thio]propyl]-3-methyl-2-thienyl]carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



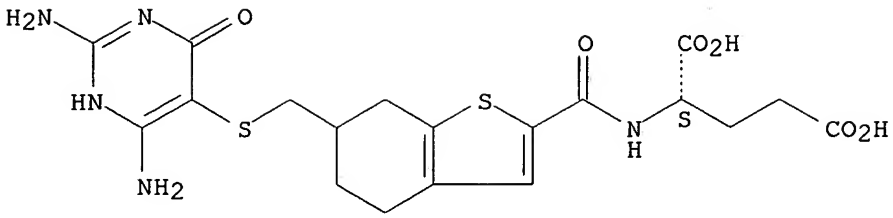
RN 160743-71-5 CAPLUS
CN L-Glutamic acid, N-[[5-[3-[(2,6-diamino-1,4-dihydro-4-oxo-5-pyrimidinyl)thio]propyl]-4-methyl-2-thienyl]carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



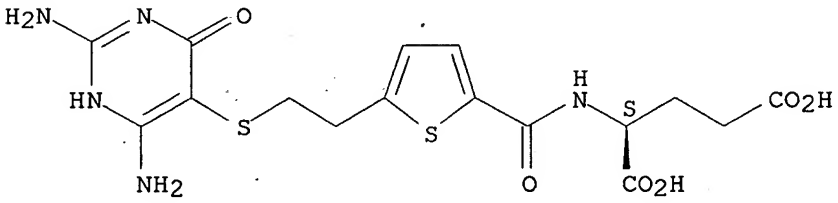
RN 160743-72-6 CAPLUS
CN L-Glutamic acid, N-[[6-[[(2,6-diamino-1,4-dihydro-4-oxo-5-pyrimidinyl)thio]methyl]-4,5,6,7-tetrahydrobenzo[b]thien-2-yl]carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

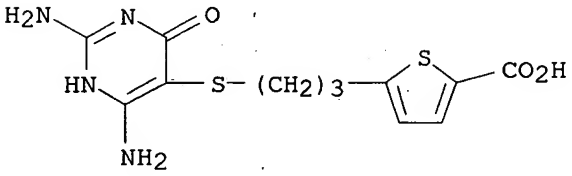


RN 160743-73-7 CAPLUS
CN L-Glutamic acid, N-[[5-[2-[(2,6-diamino-1,4-dihydro-4-oxo-5-pyrimidinyl)thio]ethyl]-2-thienyl]carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

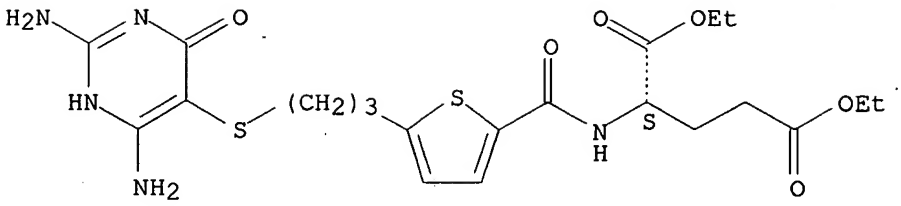


IT **160743-83-9P 160743-86-2P 160743-99-7P**
160744-03-6P 160744-09-2P 160744-10-5P
160744-17-2P 160744-18-3P 160744-19-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of substituted thiapyrimidinone and selenopyrimidinone derivs. as antiproliferative agents)
RN 160743-83-9 CAPLUS
CN 2-Thiophenecarboxylic acid, 5-[3-[(2,6-diamino-1,4-dihydro-4-oxo-5-pyrimidinyl)thio]propyl]- (9CI) (CA INDEX NAME)



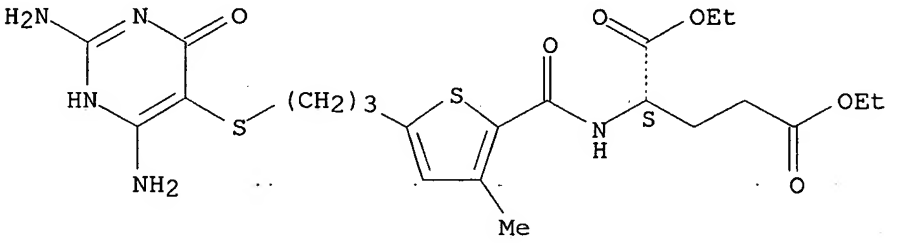
RN 160743-86-2 CAPLUS
CN L-Glutamic acid, N-[[5-[3-[(2,6-diamino-1,4-dihydro-4-oxo-5-pyrimidinyl)thio]propyl]-2-thienyl]carbonyl]-, diethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

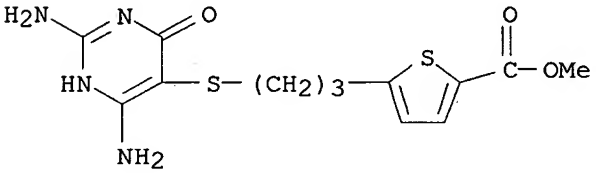


RN 160743-99-7 CAPLUS
CN L-Glutamic acid, N-[[5-[3-[(2,6-diamino-1,4-dihydro-4-oxo-5-pyrimidinyl)thio]propyl]-3-methyl-2-thienyl]carbonyl]-, diethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

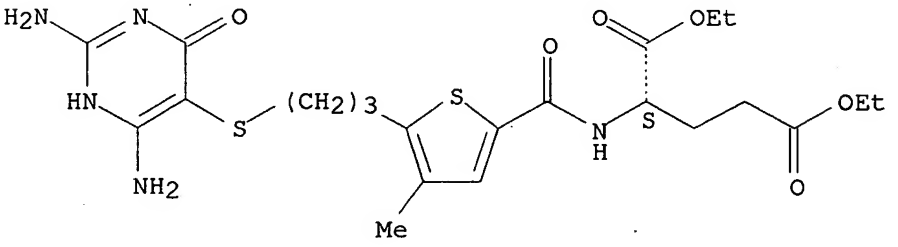


RN 160744-03-6 CAPLUS
CN 2-Thiophenecarboxylic acid, 5-[3-[(2,6-diamino-1,4-dihydro-4-oxo-5-pyrimidinyl)thio]propyl]-, methyl ester (9CI) (CA INDEX NAME)



RN 160744-09-2 CAPLUS
CN L-Glutamic acid, N-[[5-[3-[(2,6-diamino-1,4-dihydro-4-oxo-5-pyrimidinyl)thio]propyl]-4-methyl-2-thienyl]carbonyl]-, diethyl ester (9CI) (CA INDEX NAME)

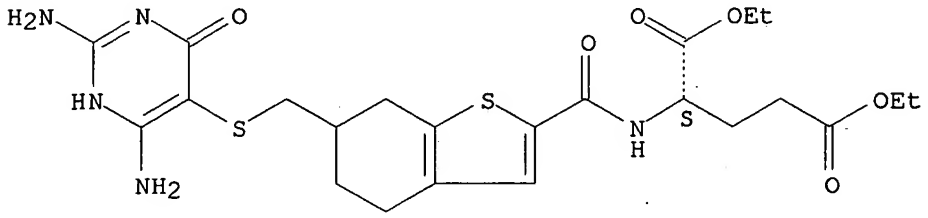
Absolute stereochemistry.



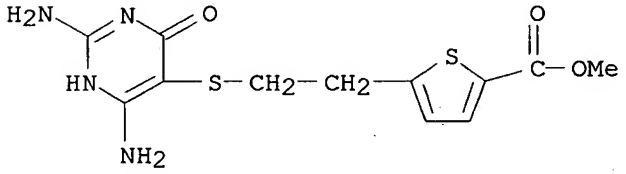
RN 160744-10-5 CAPLUS

CN L-Glutamic acid, N-[[6-[[(2,6-diamino-1,4-dihydro-4-oxo-5-pyrimidinyl)thio]methyl]-4,5,6,7-tetrahydrobenzo[b]thien-2-yl]carbonyl]-, diethyl ester (9CI) (CA INDEX NAME)

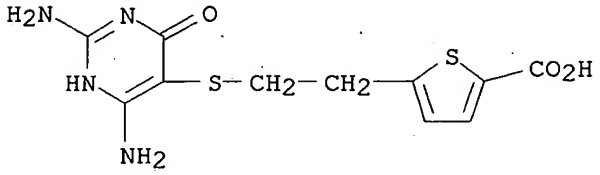
Absolute stereochemistry.



RN 160744-17-2 CAPLUS
CN 2-Thiophenecarboxylic acid, 5-[2-[(2,6-diamino-1,4-dihydro-4-oxo-5-pyrimidinyl)thio]ethyl]-, methyl ester (9CI) (CA INDEX NAME)

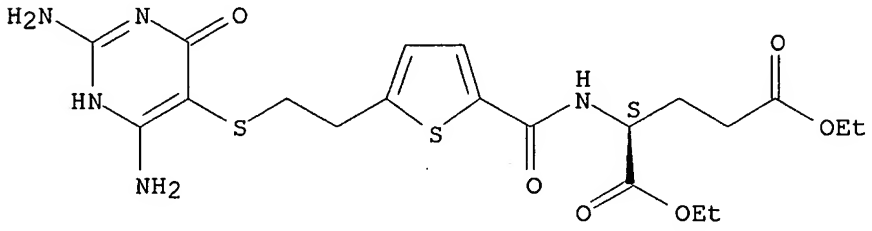


RN 160744-18-3 CAPLUS
CN 2-Thiophenecarboxylic acid, 5-[2-[(2,6-diamino-1,4-dihydro-4-oxo-5-pyrimidinyl)thio]ethyl]- (9CI) (CA INDEX NAME)



RN 160744-19-4 CAPLUS
CN L-Glutamic acid, N-[[5-[2-[(2,6-diamino-1,4-dihydro-4-oxo-5-pyrimidinyl)thio]ethyl]-2-thienyl]carbonyl]-, diethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

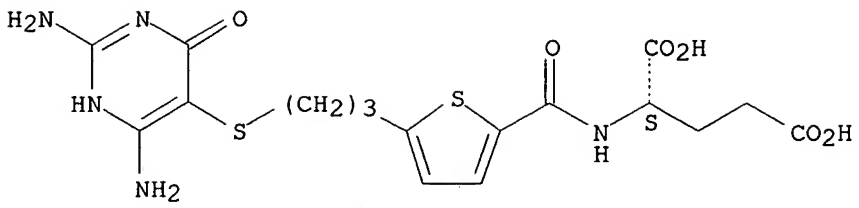


L4 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2002 ACS
AN 1998:180586 CAPLUS
DN 128:217629
TI Preparation of antiproliferative 5-thiapyrimidinone and 5-selenopyrimidinone glutamate compounds
IN Varney, Michael D.; Romines, William H.; Palmer, Cynthia L.; Deal, Judith G.
PA Agouron Pharmaceuticals, Inc., USA
SO U.S., 21 pp., Cont.-in-part of U.S. Ser. No. 991,259, abandoned.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 3

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 5726312	A	19980310	US 1995-449602	19950524
	CA 2151588	AA	19940623	CA 1993-2151588	19931210
	ES 2145122	T3	20000701	ES 1994-904399	19931210
	US 6207670	B1	20010327	US 2000-588654	20000607
PRAI	US 1992-991259	B2	19921216		
	US 1998-3163	A3	19980106		
	US 1999-307595	A3	19990510		

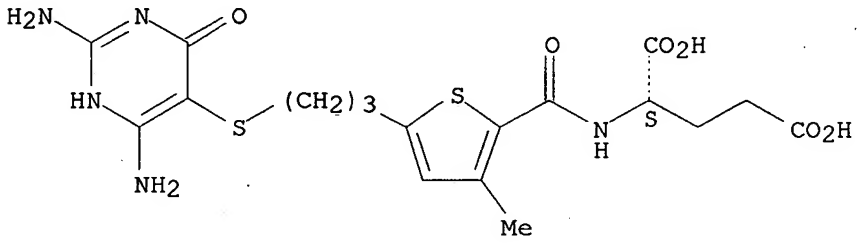
OS MARPAT 128:217629
AB Title compds. [I; A = S, Se; Z = (un)substituted noncyclic spacer contg. 1-10 atoms, (un)substituted mono-, fused, or polycarbocyclic or heterocyclic radical, etc.; R3 = H, (un)branched, (un)substituted C1-6 alkyl or C3-6 cycloalkyl; R4 = OH, C1-6 alkoxy, optionally contg. one or more OH or amino groups, (un)protected amino acid group], or pharmaceutically acceptable salts were prepd. as glycinamide ribonucleotide formyl transferase (GARFT) and AICARFT inhibitors. Thus, 5-bromo-2,6-diamino-4(3H)-pyrimidinone (prepn. given) was heated with Me 4-(3-thiopropyl)benzoate (prepn. given) and diisopropylethylamine in DMF at 100.degree. to give 73% Me 4-[3-[2,6-diamino-4(3H)-oxopyrimidin-5-yl]thiopropyl]benzoate. This was sapond. (91.6%) and the acid was coupled with L-glutamic acid di-Et ester hydrochloride using 4-methylmorpholine and Ph N-phenylphosphoroamidochloridate in 1-methyl-2-pyrrolidinone to give the amide diester, which was sapond. to give title compd. II. The latter showed IC50 = 0.079 .mu.M for inhibition of L1210 murine leukemia, and inhibited GARFT with Ki = 0.11 .mu.M.
IT **160743-67-9P 160743-70-4P 160743-71-5P 160743-72-6P 160743-73-7P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of antiproliferative thiapyrimidinone and selenopyrimidinone glutamate compds.)
RN 160743-67-9 CAPLUS
CN L-Glutamic acid, N-[[5-[3-[(2,6-diamino-1,4-dihydro-4-oxo-5-pyrimidinyl)thio]propyl]-2-thienyl]carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



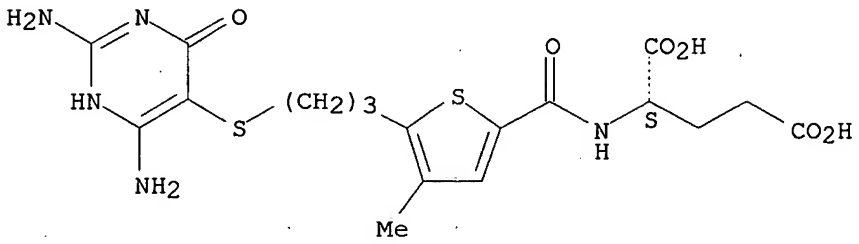
RN 160743-70-4 CAPLUS
CN L-Glutamic acid, N-[[5-[3-[(2,6-diamino-1,4-dihydro-4-oxo-5-pyrimidinyl)thio]propyl]-3-methyl-2-thienyl]carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



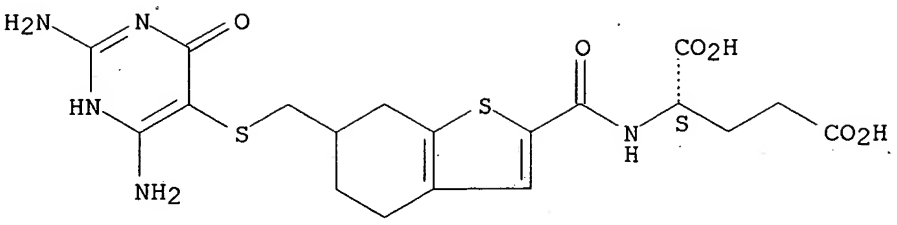
RN 160743-71-5 CAPLUS
CN L-Glutamic acid, N-[[5-[3-[(2,6-diamino-1,4-dihydro-4-oxo-5-pyrimidinyl)thio]propyl]-4-methyl-2-thienyl]carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



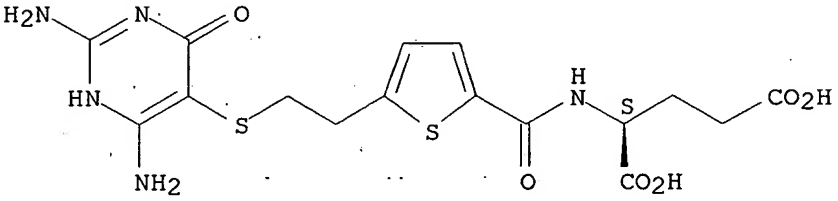
RN 160743-72-6 CAPLUS
CN L-Glutamic acid, N-[[6-[[(2,6-diamino-1,4-dihydro-4-oxo-5-pyrimidinyl)thio]methyl]-4,5,6,7-tetrahydrobenzo[b]thien-2-yl]carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

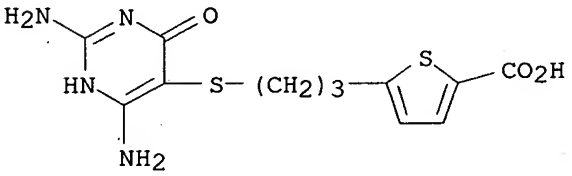


RN 160743-73-7 CAPLUS
CN L-Glutamic acid, N-[[5-[2-[(2,6-diamino-1,4-dihydro-4-oxo-5-pyrimidinyl)thio]ethyl]-2-thienyl]carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

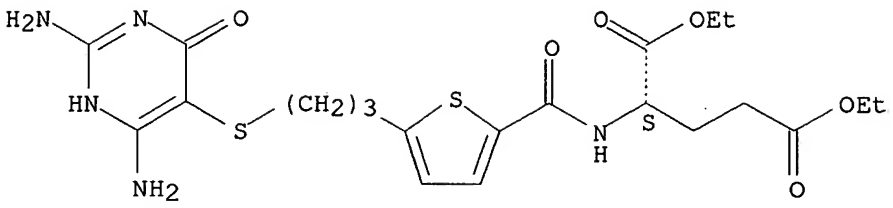


IT **160743-83-9P 160743-86-2P 160743-99-7P**
160744-03-6P 160744-09-2P 160744-10-5P
160744-17-2P 160744-18-3P 160744-19-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of antiproliferative thiapyrimidinone and selenopyrimidinone glutamate compds.)
RN 160743-83-9 CAPLUS
CN 2-Thiophenecarboxylic acid, 5-[3-[(2,6-diamino-1,4-dihydro-4-oxo-5-pyrimidinyl)thio]propyl]- (9CI) (CA INDEX NAME)



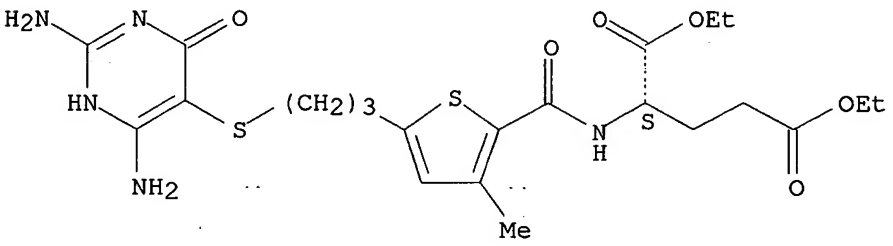
RN 160743-86-2 CAPLUS
CN L-Glutamic acid, N-[[5-[3-[(2,6-diamino-1,4-dihydro-4-oxo-5-pyrimidinyl)thio]propyl]-2-thienyl]carbonyl]-, diethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

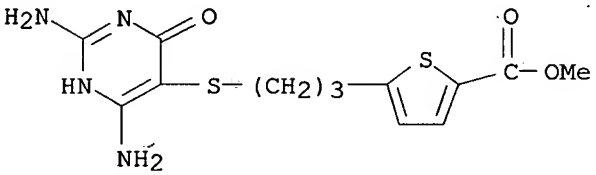


RN 160743-99-7 CAPLUS
CN L-Glutamic acid, N-[[5-[3-[(2,6-diamino-1,4-dihydro-4-oxo-5-pyrimidinyl)thio]propyl]-3-methyl-2-thienyl]carbonyl]-, diethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

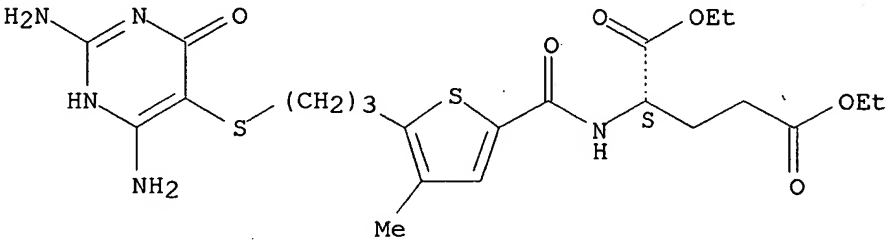


RN 160744-03-6 CAPLUS
CN 2-Thiophenecarboxylic acid, 5-[3-[(2,6-diamino-1,4-dihydro-4-oxo-5-pyrimidinyl)thio]propyl]-, methyl ester (9CI) (CA INDEX NAME)



RN 160744-09-2 CAPLUS
CN L-Glutamic acid, N-[[5-[3-[(2,6-diamino-1,4-dihydro-4-oxo-5-pyrimidinyl)thio]propyl]-4-methyl-2-thienyl]carbonyl]-, diethyl ester (9CI) (CA INDEX NAME)

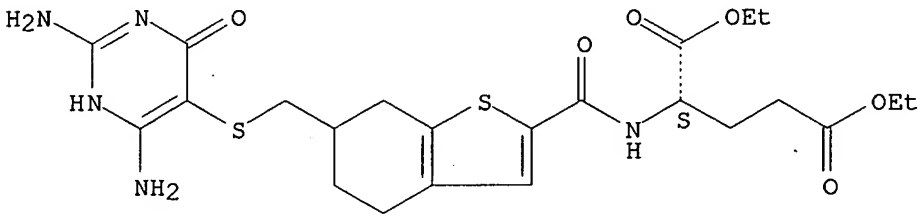
Absolute stereochemistry.



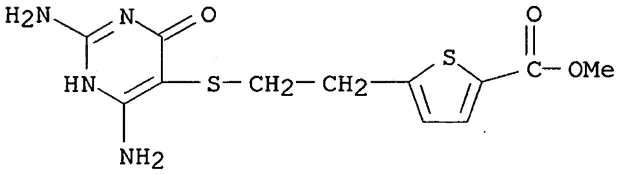
RN 160744-10-5 CAPLUS

CN L-Glutamic acid, N-[[6-[[(2,6-diamino-1,4-dihydro-4-oxo-5-pyrimidinyl)thio]methyl]-4,5,6,7-tetrahydrobenzo[b]thien-2-yl]carbonyl]-, diethyl ester (9CI) (CA INDEX NAME)

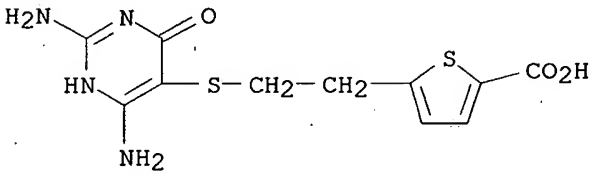
Absolute stereochemistry.



RN 160744-17-2 CAPLUS
CN 2-Thiophenecarboxylic acid, 5-[2-[(2,6-diamino-1,4-dihydro-4-oxo-5-pyrimidinyl)thio]ethyl]-, methyl ester (9CI) (CA INDEX NAME)

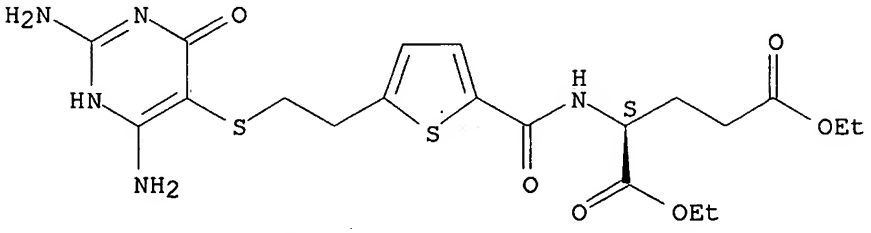


RN 160744-18-3 CAPLUS
CN 2-Thiophenecarboxylic acid, 5-[2-[(2,6-diamino-1,4-dihydro-4-oxo-5-pyrimidinyl)thio]ethyl]- (9CI) (CA INDEX NAME)

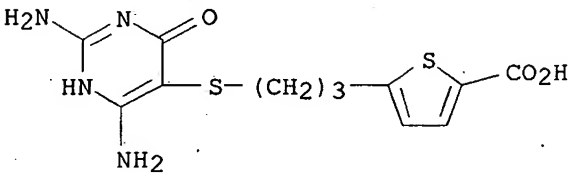


RN 160744-19-4 CAPLUS
CN L-Glutamic acid, N-[[5-[2-[(2,6-diamino-1,4-dihydro-4-oxo-5-pyrimidinyl)thio]ethyl]-2-thienyl]carbonyl]-, diethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

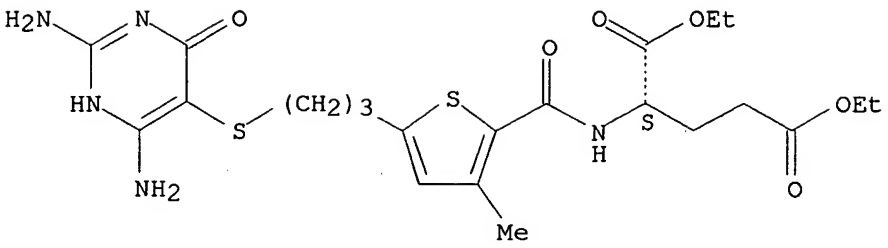


L4 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2002 ACS
AN 1997:528436 CAPLUS
DN 127:130445
TI Protein Structure-Based Design, Synthesis, and Biological Evaluation of 5-Thia-2,6-diamino-4(3H)-oxopyrimidines: Potent Inhibitors of Glycinamide Ribonucleotide Transformylase with Potent Cell Growth Inhibition
AU Varney, Michael D.; Palmer, Cindy L.; Romines, William H., III; Boritzki, Theodore; Margosiak, Stephen A.; Almassy, Robert; Janson, Cheryl A.; Bartlett, Charlotte; Howland, Eleanor J.; Ferre, Rosanne
CS Agouron Pharmaceuticals Inc., San Diego, CA, 92121, USA
SO Journal of Medicinal Chemistry (1997), 40(16), 2502-2524
CODEN: JMCMAR; ISSN: 0022-2623
PB American Chemical Society
DT Journal
LA English
AB The design, synthesis, biochem., and biol. evaluation of a novel series of 5-thia-2,6-diamino-4(3H)-oxopyrimidine inhibitors of glycinamide ribonucleotide transformylase (GART) are described. The compds. were designed using the X-ray crystal structure of human GART. The monocyclic 5-thiapyrimidinones were synthesized by coupling an alkyl thiol with 5-bromo-2,6-diamino-4(3H)-pyrimidinone. The bicyclic compds. were prepd. in both racemic and diastereomerically pure forms using two distinct synthetic routes. The compds. were found to have human GART Kis ranging from 30 .mu.M to 2 nM. The compds. inhibited the growth of both L1210 and CCRF-CEM cells in culture with potencies down to the low nanomolar range and were found to be selective for the de novo purine biosynthesis pathway. The most potent inhibitors had 2,5-disubstituted thiophene rings attached to the glutamate moiety. Placement of a Me substituent at the 4-position of the thiophene ring resulted in inhibitors with significantly decreased mFBP (human folate-binding protein) affinity.
IT **160743-83-9P 160743-99-7P 160744-03-6P**
160744-09-2P 160744-10-5P 160744-17-2P
160744-18-3P 193064-83-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and reaction; thiadiaminooxopyrimidine deriv. prepn., glycinamide ribonucleotide transformylase-inhibiting activity, and antitumor activity)
RN 160743-83-9 CAPLUS
CN 2-Thiophenecarboxylic acid, 5-[3-[(2,6-diamino-1,4-dihydro-4-oxo-5-pyrimidinyl)thio]propyl]- (9CI) (CA INDEX NAME)

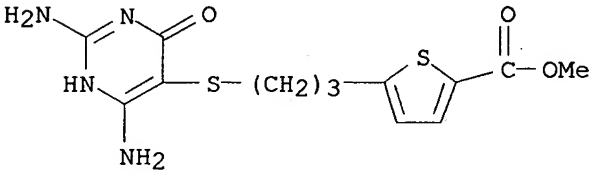


RN 160743-99-7 CAPLUS
CN L-Glutamic acid, N-[[5-[3-[(2,6-diamino-1,4-dihydro-4-oxo-5-pyrimidinyl)thio]propyl]-3-methyl-2-thienyl]carbonyl]-, diethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

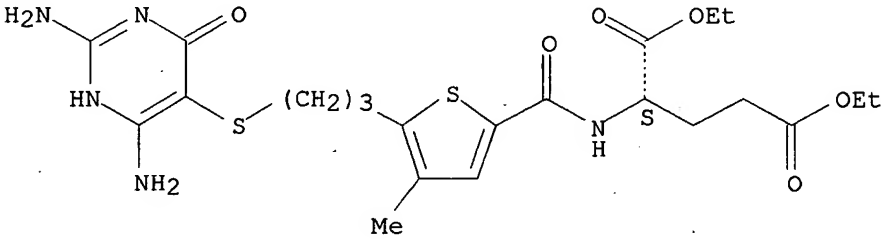


RN 160744-03-6 CAPLUS
CN 2-Thiophenecarboxylic acid, 5-[3-[(2,6-diamino-1,4-dihydro-4-oxo-5-pyrimidinyl)thio]propyl]-, methyl ester (9CI) (CA INDEX NAME)



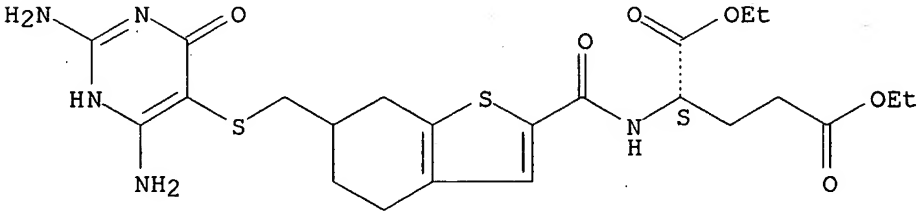
RN 160744-09-2 CAPLUS
CN L-Glutamic acid, N-[[5-[3-[(2,6-diamino-1,4-dihydro-4-oxo-5-pyrimidinyl)thio]propyl]-4-methyl-2-thienyl]carbonyl]-, diethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



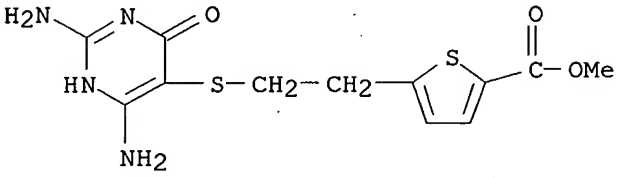
RN 160744-10-5 CAPLUS
CN L-Glutamic acid, N-[[6-[[(2,6-diamino-1,4-dihydro-4-oxo-5-pyrimidinyl)thio]methyl]-4,5,6,7-tetrahydrobenzo[b]thien-2-yl]carbonyl]-, diethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

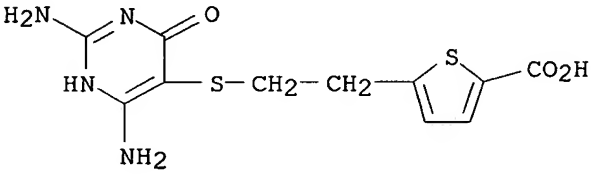


RN 160744-17-2 CAPLUS

CN 2-Thiophenecarboxylic acid, 5-[2-[(2,6-diamino-1,4-dihydro-4-oxo-5-pyrimidinyl)thio]ethyl]-, methyl ester (9CI) (CA INDEX NAME)

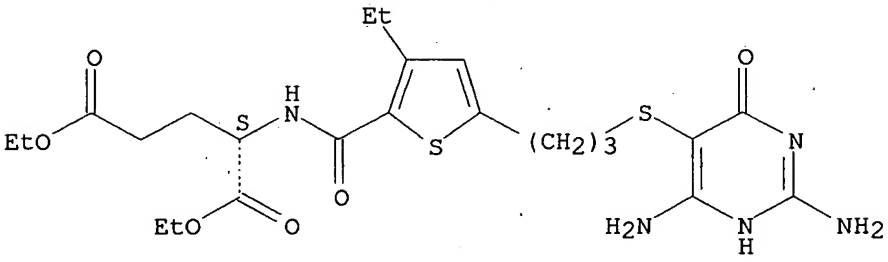


RN 160744-18-3 CAPLUS
CN 2-Thiophenecarboxylic acid, 5-[2-[(2,6-diamino-1,4-dihydro-4-oxo-5-pyrimidinyl)thio]ethyl]- (9CI) (CA INDEX NAME)



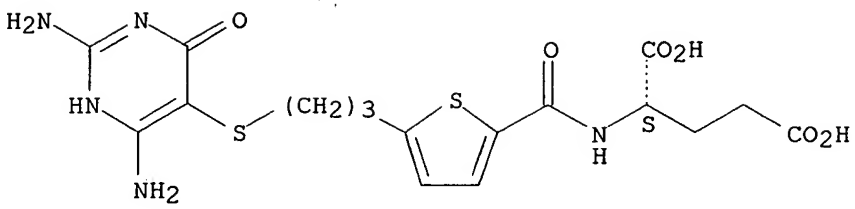
RN 193064-83-4 CAPLUS
CN L-Glutamic acid, N-[[5-[3-[(2,6-diamino-1,4-dihydro-4-oxo-5-pyrimidinyl)thio]propyl]-3-ethyl-2-thienyl]carbonyl]-, diethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



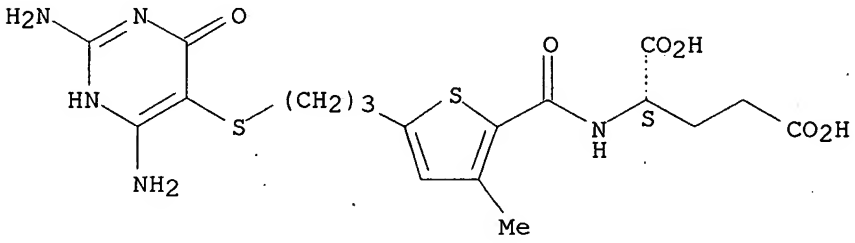
IT **160743-67-9P 160743-70-4P 160743-71-5P**
160743-72-6P 160743-73-7P 193064-85-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(thiadiaminooxopyrimidine deriv. prepn., glycinamide ribonucleotide transformylase-inhibiting activity, and antitumor activity)
RN 160743-67-9 CAPLUS
CN L-Glutamic acid, N-[[5-[3-[(2,6-diamino-1,4-dihydro-4-oxo-5-pyrimidinyl)thio]propyl]-2-thienyl]carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



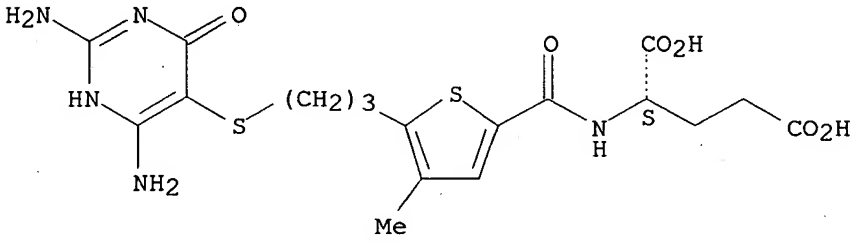
RN 160743-70-4 CAPLUS
CN L-Glutamic acid, N-[[5-[3-[(2,6-diamino-1,4-dihydro-4-oxo-5-pyrimidinyl)thio]propyl]-3-methyl-2-thienyl]carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



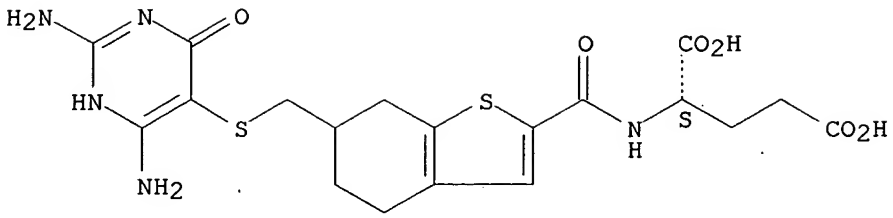
RN 160743-71-5 CAPLUS
CN L-Glutamic acid, N-[[5-[3-[(2,6-diamino-1,4-dihydro-4-oxo-5-pyrimidinyl)thio]propyl]-4-methyl-2-thienyl]carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



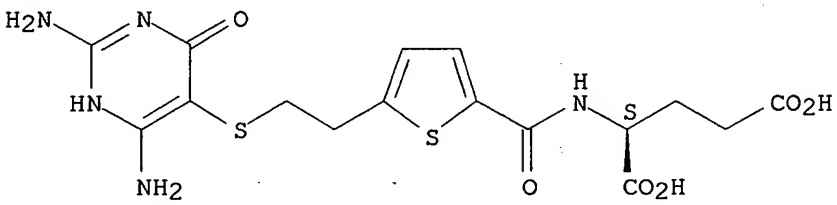
RN 160743-72-6 CAPLUS
CN L-Glutamic acid, N-[[6-[[(2,6-diamino-1,4-dihydro-4-oxo-5-pyrimidinyl)thio]methyl]-4,5,6,7-tetrahydrobenzo[b]thien-2-yl]carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



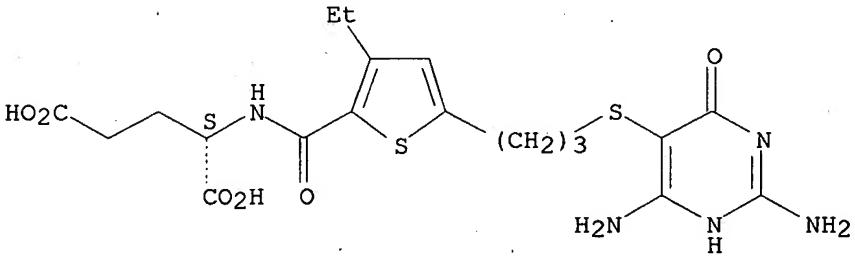
RN 160743-73-7 CAPLUS
CN L-Glutamic acid, N-[[5-[2-[(2,6-diamino-1,4-dihydro-4-oxo-5-pyrimidinyl)thio]ethyl]-2-thienyl]carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



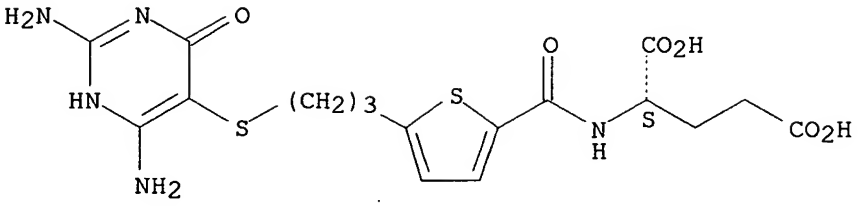
RN 193064-85-6 CAPLUS
CN L-Glutamic acid, N-[[5-[3-[(2,6-diamino-1,4-dihydro-4-oxo-5-pyrimidinyl)thio]propyl]-3-ethyl-2-thienyl]carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



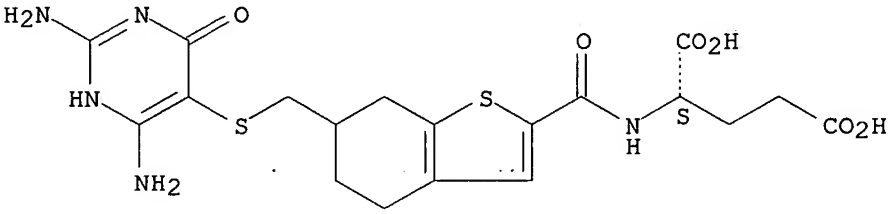
IT **160743-67-9D**, glycinamide ribonucleotide transformylase complexes
160743-72-6D, glycinamide ribonucleotide transformylase complexes
RL: PRP (Properties)
(thiadiaminooxopyrimidine deriv. prepn., glycinamide ribonucleotide transformylase-inhibiting activity, and antitumor activity)
RN 160743-67-9 CAPLUS
CN L-Glutamic acid, N-[[5-[3-[(2,6-diamino-1,4-dihydro-4-oxo-5-pyrimidinyl)thio]propyl]-2-thienyl]carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



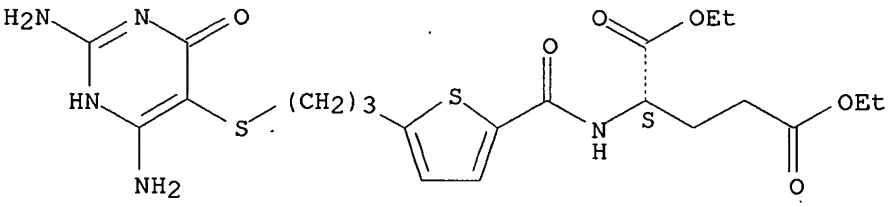
RN 160743-72-6 CAPLUS
CN L-Glutamic acid, N-[[6-[[(2,6-diamino-1,4-dihydro-4-oxo-5-pyrimidinyl)thio]methyl]-4,5,6,7-tetrahydrobenzo[b]thien-2-yl]carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



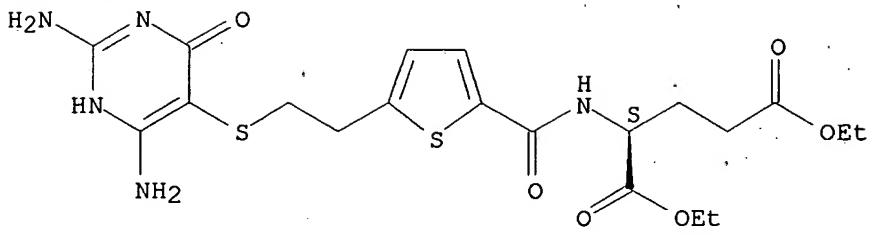
IT **160743-86-2P 160744-19-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(thiadiaminooxopyrimidine deriv. prepn., glycinamide ribonucleotide transformylase-inhibiting activity, and antitumor activity)
RN 160743-86-2 CAPLUS
CN L-Glutamic acid, N-[[5-[3-[(2,6-diamino-1,4-dihydro-4-oxo-5-pyrimidinyl)thio]propyl]-2-thienyl]carbonyl]-, diethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 160744-19-4 CAPLUS
CN L-Glutamic acid, N-[[5-[2-[(2,6-diamino-1,4-dihydro-4-oxo-5-pyrimidinyl)thio]ethyl]-2-thienyl]carbonyl]-, diethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2002 ACS
AN 1995:339381 CAPLUS
DN 122:106522
TI Preparation of antiproliferative 5-thiapyrimidinone and 5-selenopyrimidinone glutamate compounds
IN Deal, Judith G.; Varney, Michael D.; Romines, William H.; Palmer, Cynthia L.
PA Agouron Pharmaceuticals, Inc., USA
SO PCT Int. Appl., 87 pp.
CODEN: PIXXD2
DT Patent
LA English

Applicant's

FAN.CNT 3

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9413295	A1	19940623	WO 1993-US11795	19931210
	W: AT, AU, BB, BG, BR, BY, CA, CH, CZ, DE, DK, ES, FI, GB, HU, JP, KP, KR, KZ, LK, LU, LV, MG, MN, MW, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SK, UA, US, UZ, VN				
	RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
	CA 2151588	AA	19940623	CA 1993-2151588	19931210
	AU 9458464	A1	19940704	AU 1994-58464	19931210
	EP 674516	A1	19951004	EP 1994-904399	19931210
	EP 674516	B1	20000202		
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	JP 08504765	T2	19960521	JP 1993-514288	19931210
	AT 189390	E	20000215	AT 1994-904399	19931210
	ES 2145122	T3	20000701	ES 1994-904399	19931210
	US 5739141	A	19980414	US 1995-448556	19950607
	US 6207670	B1	20010327	US 2000-588654	20000607
	US 2001018443	A1	20010830	US 2001-782284	20010214
	US 6323210	B2	20011127		
PRAI	US 1992-991259	A	19921216		
	WO 1993-US11795	W	19931210		
	US 1995-448556	A3	19950607		
	US 1998-3163	A3	19980106		
	US 1999-307595	A3	19990510		
	US 2000-588654	A3	20000607		

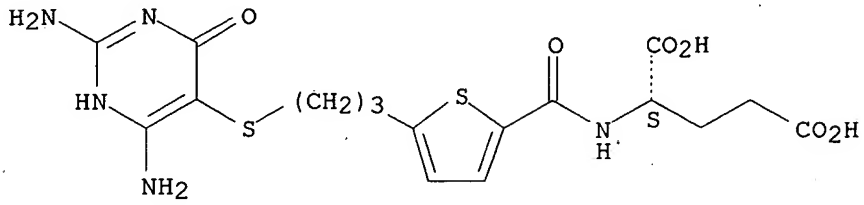
AB Title compds. [I; A = S, Se; Z = (substituted) noncyclic spacer, carbocyclic or heterocyclic radical, etc.; R1, R2 = H, alkyl, other readily lyzable groups; R3 = H, (substituted) alkyl], were prepd. Thus, 5-bromo-2,6-diamino-4(3H)-pyrimidinone (prepn. given) was heated with Me 4-(3-thiopropyl)benzoate (prepn. given) and diisopropylethylamine in DMF at 100.degree. to give 73% Me 4-[3-[2,6-diamino-4(3H)-oxopyrimidin-5-yl]thiopropyl]benzoate. The latter was sapond. (91.6%) and the acid was coupled with S-glutamic acid di-Et ester hydrochloride using 4-methylmorpholine and Ph N-phenylphosphoroamidochloridate in 1-methyl-2-pyrrolidinone to give the amide diester, which was sapond. to give title compd. II. The latter showed IC50 = 0.079 .mu.M for inhibition of L1210 murine leukemia, and inhibited glycinamide ribonucleotide formyl transferase with Ki = 0.11 .mu.M.

IT **160743-67-9P 160743-70-4P 160743-71-5P 160743-72-6P 160743-73-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as antiproliferative)

RN 160743-67-9 CAPLUS
CN L-Glutamic acid, N-[[5-[3-[(2,6-diamino-1,4-dihydro-4-oxo-5-

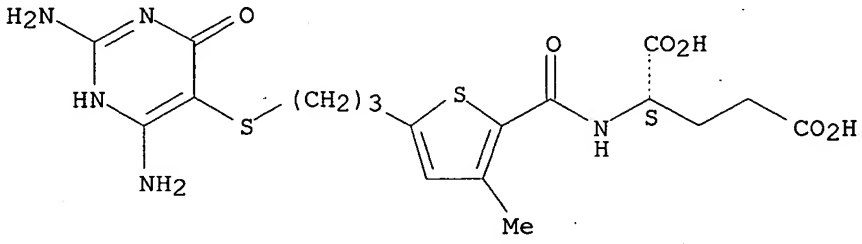
pyrimidinyl)thio]propyl]-2-thienyl]carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



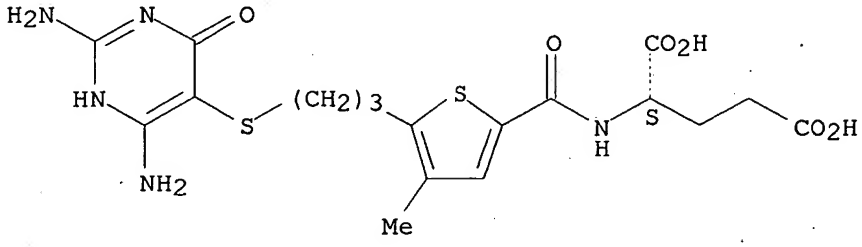
RN 160743-70-4 CAPLUS
CN L-Glutamic acid, N-[[5-[3-[(2,6-diamino-1,4-dihydro-4-oxo-5-pyrimidinyl)thio]propyl]-3-methyl-2-thienyl]carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



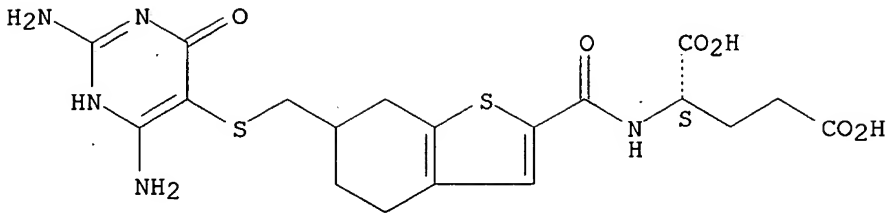
RN 160743-71-5 CAPLUS
CN L-Glutamic acid, N-[[5-[3-[(2,6-diamino-1,4-dihydro-4-oxo-5-pyrimidinyl)thio]propyl]-4-methyl-2-thienyl]carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



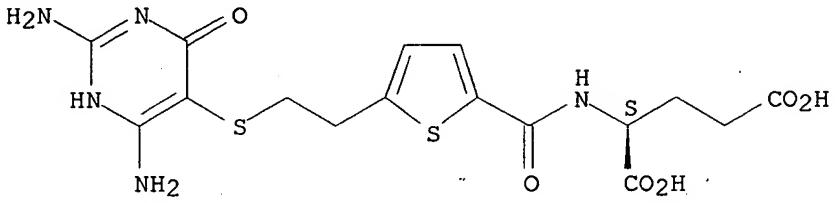
RN 160743-72-6 CAPLUS
CN L-Glutamic acid, N-[[6-[[(2,6-diamino-1,4-dihydro-4-oxo-5-pyrimidinyl)thio]methyl]-4,5,6,7-tetrahydrobenzo[b]thien-2-yl]carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

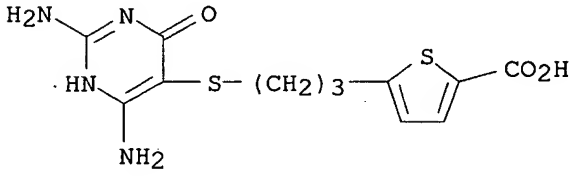


RN 160743-73-7 CAPLUS
CN L-Glutamic acid, N-[[5-[2-[(2,6-diamino-1,4-dihydro-4-oxo-5-pyrimidinyl)thio]ethyl]-2-thienyl]carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

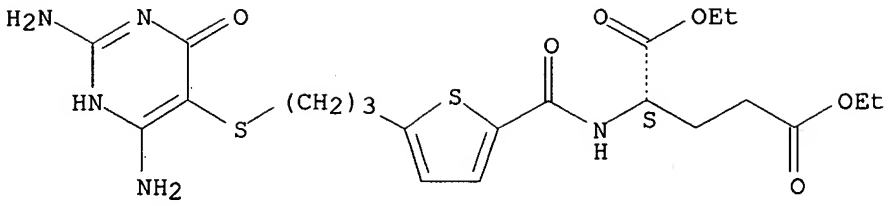


IT **160743-83-9P 160743-86-2P 160743-99-7P**
160744-03-6P 160744-09-2P 160744-10-5P
160744-17-2P 160744-18-3P 160744-19-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as intermediate for antiproliferative)
RN 160743-83-9 CAPLUS
CN 2-Thiophenecarboxylic acid, 5-[3-[(2,6-diamino-1,4-dihydro-4-oxo-5-pyrimidinyl)thio]propyl]- (9CI) (CA INDEX NAME)



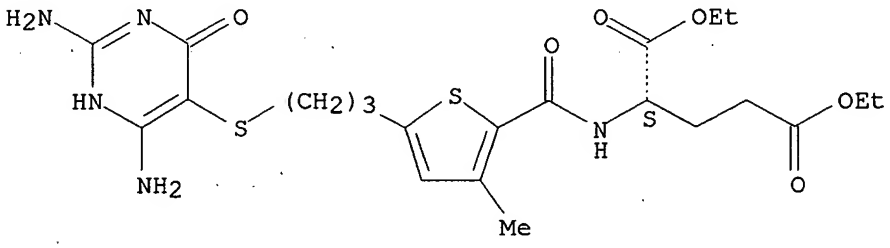
RN 160743-86-2 CAPLUS
CN L-Glutamic acid, N-[[5-[3-[(2,6-diamino-1,4-dihydro-4-oxo-5-pyrimidinyl)thio]propyl]-2-thienyl]carbonyl]-, diethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

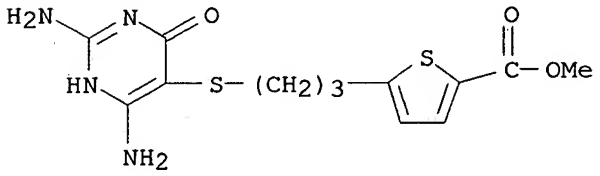


RN 160743-99-7 CAPLUS
CN L-Glutamic acid, N-[[5-[3-[(2,6-diamino-1,4-dihydro-4-oxo-5-pyrimidinyl)thio]propyl]-3-methyl-2-thienyl]carbonyl]-, diethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

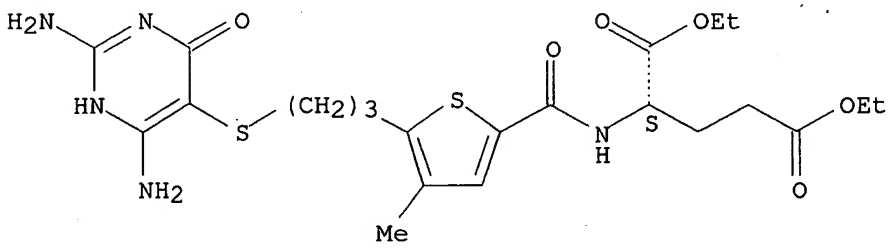


RN 160744-03-6 CAPLUS
CN 2-Thiophenecarboxylic acid, 5-[3-[(2,6-diamino-1,4-dihydro-4-oxo-5-pyrimidinyl)thio]propyl]-, methyl ester (9CI) (CA INDEX NAME)



RN 160744-09-2 CAPLUS
CN L-Glutamic acid, N-[[5-[3-[(2,6-diamino-1,4-dihydro-4-oxo-5-pyrimidinyl)thio]propyl]-4-methyl-2-thienyl]carbonyl]-, diethyl ester (9CI) (CA INDEX NAME)

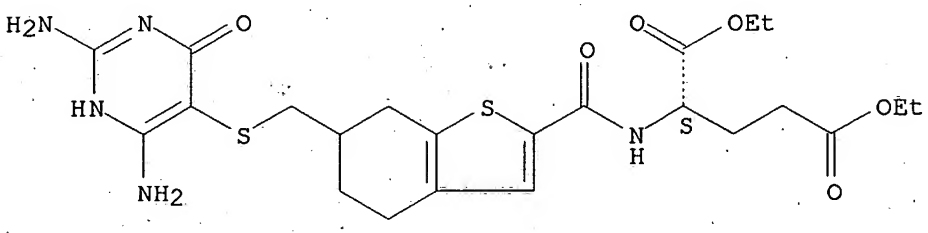
Absolute stereochemistry.



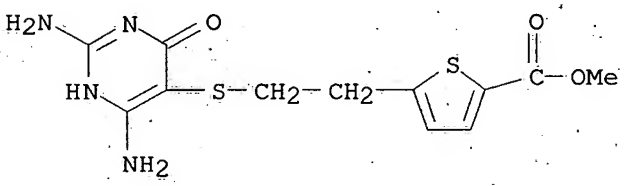
RN 160744-10-5 CAPLUS

CN L-Glutamic acid, N-[[6-[[(2,6-diamino-1,4-dihydro-4-oxo-5-pyrimidinyl)thio]methyl]-4,5,6,7-tetrahydrobenzo[b]thien-2-yl]carbonyl]-, diethyl ester (9CI) (CA INDEX NAME)

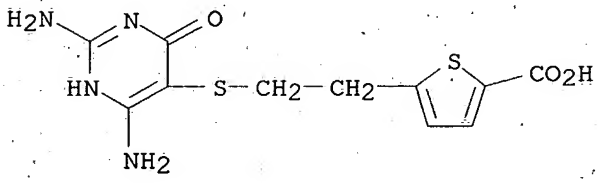
Absolute stereochemistry.



RN 160744-17-2 CAPLUS
CN 2-Thiophenecarboxylic acid, 5-[2-[(2,6-diamino-1,4-dihydro-4-oxo-5-pyrimidinyl)thio]ethyl]-, methyl ester (9CI) (CA INDEX NAME)

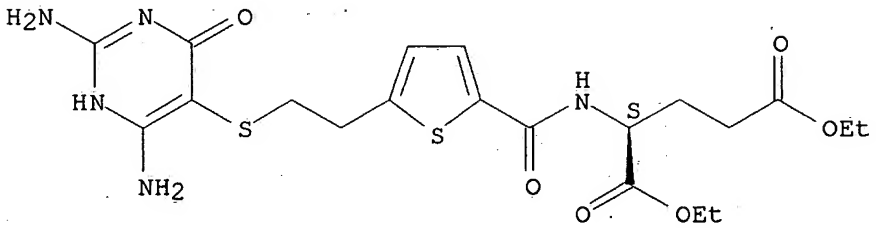


RN 160744-18-3 CAPLUS
CN 2-Thiophenecarboxylic acid, 5-[2-[(2,6-diamino-1,4-dihydro-4-oxo-5-pyrimidinyl)thio]ethyl]- (9CI) (CA INDEX NAME)



RN 160744-19-4 CAPLUS
CN L-Glutamic acid, N-[[5-[2-[(2,6-diamino-1,4-dihydro-4-oxo-5-pyrimidinyl)thio]ethyl]-2-thienyl]carbonyl]-, diethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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L2              1 S L1 SSS SAM
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L4              5 S L3

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=> s l3
L5              0 L3

=> log y
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FULL ESTIMATED COST                                0.38     163.59

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)    SINCE FILE      TOTAL
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CA SUBSCRIBER PRICE                                0.00      -3.10

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